

Construction of Modified Central Composite Designs for Non-standard Models

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Received: June 19, 2018 Accepted: July 10, 2018 Online Published: August 9, 2018

doi:10.5539/ijsp.v7n5p95

URL: <https://doi.org/10.5539/ijsp.v7n5p95>

Abstract

The use of loss function in studying the reduction in determinant of information matrix due to missing observations has effectively produced designs that are robust to missing observations. Modified central composite designs are constructed for non-standard models using principles of the loss function or equivalently first compound of $(I-H)$ matrix associated with hat matrix H . Although central composite designs (CCDs) are reasonably robust to model mis-specifications, efficient designs with fewer design points are more economical. By classifying the losses due to missing design points in the CCD portions, where there are multiple losses associated with specified CCD portions, the design points having less influence may be deleted from the full CCD. This leads to a possible increase in design efficiency and offers alternative designs, similar in the structure of CCDs, for non-standard models.

Keywords: Loss Function, Missing Observation, Non-Standard Model, Central Composite Design, Design Efficiency

1. Introduction

Response surface methodology has continued to play vital roles in developing, optimizing and improving processes, particularly where several input variables, $\xi_1, \xi_2, \dots, \xi_k$, potentially influence some performance measure or quality characteristic, y , of the process under study. The relationship between the input variables and the response variable is

$$y = f(\xi_1, \xi_2, \dots, \xi_k) + \varepsilon \quad (1)$$

where ε is the random error component assumed to have a normal distribution with zero mean and constant variance such that

$$E(y) = f(\xi_1, \xi_2, \dots, \xi_k) = \eta \quad (2)$$

In most practical situations, the true response function is unknown but may be approximated using low-degree polynomials in some relatively small region of the independent variable space.

For convenience, the natural input variables $\xi_1, \xi_2, \dots, \xi_k$ are usually transformed to dimensionless coded variables x_1, x_2, \dots, x_k .

When first-order model is considered adequate, it is assumed that there is little or no indication of the presence of curvature in the response function. In terms of the coded input variables, the first-order model is

$$\eta = \hat{\beta}_0 + \sum_{i=1}^k \hat{\beta}_i x_i \quad (3)$$

However, if there is an indication of interaction between the independent variables, the first-order model with a measure of interaction is

$$\eta = \hat{\beta}_0 + \sum_{i=1}^k \hat{\beta}_i x_i + \sum_{i < j} \hat{\beta}_{ij} x_i x_j \quad (4)$$

Model inadequacy exists when there is substantial curvature in the true response function (indicated by the lack of fit of first-order model) and the need for an approximating polynomial of higher order arises.

In terms of the coded input variables, the second-order model is

$$\eta = \hat{\beta}_0 + \sum_{i=1}^k \hat{\beta}_i x_i + \sum_{i < j} \hat{\beta}_{ij} x_i x_j + \sum_{i=1}^k \hat{\beta}_{ii} x_i^2 \quad (5)$$

$\hat{\beta}$'s represent the model parameter estimates obtained using the method of least squares.

As conventionally used, the estimated response, in matrix form, is

$$\hat{y} = X\hat{\beta}$$

where the least squares estimate of vector of the unknown parameters β is

$$\hat{\beta} = (X'X)^{-1} X'y$$

The unknown parameters are estimated on the basis of N uncorrelated observations.

y denotes the vector of observations and X denotes the model matrix. It is assumed that the information matrix $X'X$ is non-singular. From the least squares estimates of the unknown parameters, the estimated response is

$$\hat{y} = X(X'X)^{-1} X'y = Hy \quad (6)$$

where $H = X(X'X)^{-1} X'$ is called the hat matrix and puts the "hat" on the vector of fitted or estimated value. One major role of the hat matrix in modeling problems is to identify observations that have greater impacts on the estimation of model parameters and fitted values. Identifying and dealing with such observations help improve statistical inferences.

Many practical situations show that approximating polynomials of second-order works well. However sometimes, not all terms in the full second-order model may be statistically significant, thus resulting in reduced models referred to as Non-standard models (Myer et al. 2009; pg 395). One of the most popularly used second-order response surface designs is the central composite design, which has factorial, axial and center portions. Other second-order response surface designs include the Box-Behnken design, Hoke design, Koshal design, Hybrid design, etc.

Our research problem is based on the practical consideration that the central composite design is meant for a full p -parameter model where $p = (k + 1)(k + 2)/2$ for k design variables x_1, x_2, \dots, x_k . Usually, the model is assumed prior to performing the experiment but may differ at the end of experimentation.

In an ideal situation, where the model is a full parameter model, the diagonal entries of the hat matrix for a central composite design show constant diagonal elements for each portion of the CCD. After data are collected, model fitting procedure may reveal that some parameters associated with the prior response surface model are deemed insignificant and are thus removed from the model. The resulting model (reduced model) is non-standard for the CCD and retains only significant terms. In the instance of a "non-standard" model, the diagonal elements of the hat matrix may not be constant for some design points in the CCD portions. To achieve constant or near constant diagonal elements in each CCD portion as well as optimize some design properties, some less influential design points may be deleted from the design and the CCD is thus modified for the newly fitted model, otherwise called, posterior model as in Borkowski and Valeroso (1997). Changes in design's efficiency is expected for the modified CCD and that is the focus of this research work, with intent of providing designs for "non-standard" or "mis-specified" models.

2. The Hat Matrix and the Loss Function

The mention of hat matrix takes one's mind to leverage which according to Myung and Kahng (2007) is a basic component of influence in linear regression models. Each diagonal element h_{ii} of the hat matrix is called leverage and measures the extent to which the fitted regression model \hat{y}_i is attracted by the given observation or data point y_i . In essence, the i^{th} leverage h_{ii} quantifies the influence that the observation y_i has on its predicted value \hat{y}_i . The diagonal elements of the hat matrix are such that $0 \leq h_{ii} \leq 1$ and $\sum_{i=1}^N h_{ii} = p$; where N is the number of data points and p is the number of model parameters, including the intercept. Aside investigating whether one or more observations excessively influence the estimated values, the hat matrix may also be used to quantify the effect of removing one or more observations from a design. Thus, the hat matrix (through its compounds) is useful in understanding effect of missing observations in a complete data set.

Akhtar and Prescott (1986) considered the relative reduction in determinant of information matrix due to missing observations, by quantifying the effect of missing observations using the criterion of loss function. When m observations in the design are missing, the complete data set is altered and the model matrix reduces by m rows. As expected, the information matrix, $X_r'X_r$, for the reduced design will differ from the information matrix, $X'X$, for the complete design. For $m \times p$ matrix X_m , of m missing rows corresponding to the m missing observations, the information matrix may be expressed as

$$X'X = X_m'X_m + X_r'X_r$$

Post multiplying yields,

$$(X'X)(X'X)^{-1} = [(X_m'X_m) + (X_r'X_r)](X'X)^{-1}$$

This implies

$$I_p = (X_m'X_m) (X'X)^{-1} + (X_r'X_r) (X'X)^{-1}$$

where I_p is an identity matrix of order p .

By rearrangement,

$$(X_r'X_r) (X'X)^{-1} = I_p - (X_m'X_m) (X'X)^{-1}$$

Post multiplying by $(X'X)$ yields

$$\begin{aligned} (X_r'X_r) (X'X)^{-1} (X'X) &= [I_p - (X_m'X_m) (X'X)^{-1}] (X'X) \\ \Rightarrow (X_r'X_r) &= [I_p - (X_m'X_m) (X'X)^{-1}] (X'X) \end{aligned}$$

Taking determinants of both sides yield

$$|(X_r'X_r)| = |[I_p - (X_m'X_m) (X'X)^{-1}]| |(X'X)|$$

This implies

$$\frac{|(X_r'X_r)|}{|(X'X)|} = |[I_p - (X_m'X_m) (X'X)^{-1}]|$$

In Akhtar (1987), the determinant $|[I_p - (X_m'X_m) (X'X)^{-1}]|$ is called the diagonal element of the m^{th} compound of $(I-H)$ where H is the hat matrix according to the m missing observations and I represents an identity matrix of same dimension as H . Specifically, the loss function measures the relative reduction in the determinant of information matrix associated with the complete design in the presence of missing observations.

Ahmad *et al.* (2010) related $|(X_r'X_r)|$ and $|(X'X)|$ using identities on the expansion of a bordered determinant

$$|(X_r'X_r)| = |(X'X)| A_{uv\dots}$$

where $A_{uv\dots}$ is the corresponding diagonal element of the m^{th} compound of $(I-H)$ matrix and H is the symmetric matrix $X(X'X)^{-1}X'$ of order N . Specifically, the u^{th} diagonal element of the first compound of $(I-H)$ matrix is A_u ; the vu^{th} diagonal element of the second compound of $(I-H)$ matrix is A_{vu} , and so on. It is clear from Akram (2002) and Atken and Rutherford (1964) that the first compound of the matrix $(I-H)$ is the hat matrix itself. Thus, the diagonal elements of the hat matrix in addition to establishing measures of influence of design points also quantify the loss due to a single missing observation.

For m missing observations, the determinant of the complete information matrix may be obtained as

$$|(X'X)| = |(X_m'X_m)| + |(X_r'X_r)|.$$

The relative loss due to any set of m missing observations is defined as

$$l_{uv\dots} = \frac{|(X'X)| - |(X_r'X_r)|}{|(X'X)|}; \quad 0 \leq l_{uv\dots} \leq 1$$

This implies

$$l_{uv\dots} = 1 - \frac{|(X_r'X_r)|}{|(X'X)|} = 1 - A_{uv\dots} = 1 - |I - (X_m'X_m) (X'X)^{-1}| \quad (\text{See Akram; 2002})$$

For central composite designs, the determinant $|(X'X)|$ is an increasing function of the axial distance α and is maximized at $\alpha = \infty$. The values of α specifies the location of the axial point and are usually chosen to satisfy various design conditions such as rotatability and orthogonal blocking. A number of researchers have studied the loss due to a set of m missing observations over a range of α value associated with central composite designs and minimax loss designs that are robust to sets of missing observations have emerged. Some of such results include Akhtar (2001) and Akram (2002). The loss functions (or equivalently, compounds of the $(I-H)$ matrix) have thus been effectively used in studying the relative reduction in determinant of information matrix due to missing observations and has effectively produced designs that are robust to missing observations. Much study on loss function considers the second-order central composite designs differing in the number of control variables and configurations of the factorial, axial and center portions; Akhtar (1987), Akhtar (2001), Akram (2002), Ahmad and Gilmour (2010), Ahmad *et al.* (2011), Yakubu *et al.* (2014), Okon and Nsude (2015), Iwundu (2017) Akhtar (1987), Akhtar (2001), Akram (2002), Ahmad and Gilmour (2010), Ahmad *et al.* (2011), Yakubu *et al.* (2014), Okon and Nsude (2015), Iwundu (2017).

3. The Central Composite Design and Another Look at the Hat Matrix

In most practical modeling situations involving several control variables, the central composite designs have been satisfactorily used in optimization phase of experimentation. However, the second-order model which justifies the use of the central composite design is assumed prior to experimentation. After data have been collected, model fitting may reveal that not all model parameters are significant and hence the need to remove insignificant parameters from the model thus resulting in a reduced posterior model.

For a full parameter second-order model, the diagonal elements of the hat matrix reveal a unique property associated with central composite designs. The diagonal elements associated with design points in a particular CCD portion are a constant for all design points in that portion. Specifically, 2^k vertex points have constant diagonal element say, $h_{ii} = d_v$; $2k$ axial points have constant diagonal element say, $h_{ii} = d_a$ and n_c center points have constant diagonal element say, $h_{ii} = d_c$. Where fractions of full factorial designs are utilized, the property remains unchanged. This implies that the design points of a CCD portion have an equal influence in modeling. For a “non-standard” or “mis-specified” model, the associated hat matrix loses the uniqueness of its diagonal elements for the employed central composite design. This clearly shows that the design points of the CCD portion do not anymore have an equal influence in modeling. Adjustments may be made on the design to retain the unique property of its diagonal elements for the posterior “mis-specified” model, either absolutely or approximately. The choice of the words “mis-specified” or “non-standard” is on the premise that the central composite design is essentially constructed for a full parameter model.

Considering, for example, a full-parameter (10-parameter) second-order model in three control variables

$$y(x_1, x_2, x_3) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{23}x_2x_3 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \beta_{33}x_3^2 + \epsilon$$

the hat matrix associated with central composite design having 8 factorial points, 6 axial points and 1 center point, is given as

$H =$	0.7972	0.0972	0.0972	-0.1028	0.0972	-0.1028	-0.1028	0.1972	-0.0889	0.1111	-0.0889	0.1111	-0.0889	0.1111	-0.0444
	0.0972	0.7972	-0.1028	0.0972	-0.1028	0.0972	0.1972	-0.1028	0.1111	-0.0889	-0.0889	0.1111	-0.0889	0.1111	-0.0444
	0.0972	-0.1028	0.7972	0.0972	-0.1028	0.1972	0.0972	-0.1028	-0.0889	0.1111	0.1111	-0.0889	-0.0889	0.1111	-0.0444
	-0.1028	0.0972	0.0972	0.7972	0.1972	-0.1028	-0.1028	0.0972	0.1111	-0.0889	0.1111	-0.0889	-0.0889	0.1111	-0.0444
	0.0972	-0.1028	-0.1028	0.1972	0.7972	0.0972	0.0972	-0.1028	-0.0889	0.1111	-0.0889	0.1111	0.1111	-0.0889	-0.0444
	-0.1028	0.0972	0.1972	-0.1028	0.0972	0.7972	-0.1028	0.0972	0.1111	-0.0889	-0.0889	0.1111	0.1111	-0.0889	-0.0444
	-0.1028	0.1972	0.0972	-0.1028	0.0972	-0.1028	0.7972	0.0972	-0.0889	0.1111	0.1111	-0.0889	0.1111	-0.0889	-0.0444
	0.1972	-0.1028	-0.1028	0.0972	-0.1028	0.0972	0.0972	0.7972	0.1111	-0.0889	0.1111	-0.0889	0.1111	-0.0889	-0.0444
	-0.0889	0.1111	-0.0889	0.1111	-0.0889	0.1111	-0.0889	0.1111	0.5556	0.3556	-0.0444	-0.0444	-0.0444	-0.0444	0.1778
	0.1111	-0.0889	0.1111	-0.0889	0.1111	-0.0889	0.1111	-0.0889	0.3556	0.5556	-0.0444	-0.0444	-0.0444	-0.0444	0.1778
	-0.0889	-0.0889	0.1111	0.1111	-0.0889	-0.0889	0.1111	0.1111	-0.0444	-0.0444	0.5556	0.3556	-0.0444	-0.0444	0.1778
	0.1111	0.1111	-0.0889	-0.0889	0.1111	0.1111	-0.0889	-0.0889	-0.0444	-0.0444	0.3556	0.5556	-0.0444	-0.0444	0.1778
	-0.0889	-0.0889	-0.0889	-0.0889	0.1111	0.1111	0.1111	0.1111	-0.0444	-0.0444	-0.0444	-0.0444	0.5556	0.3556	0.1778
	0.1111	0.1111	0.1111	0.1111	-0.0889	-0.0889	-0.0889	-0.0889	-0.0444	-0.0444	-0.0444	-0.0444	0.3556	0.5556	0.1778
	-0.0444	-0.0444	-0.0444	-0.0444	-0.0444	-0.0444	-0.0444	-0.0444	0.1778	0.1778	0.1778	0.1778	0.1778	0.1778	0.2889

Associated with the 8 factorial points $(-1,-1,-1), (1,-1,-1), (-1,1,-1), (1,1,-1), (-1,-1,1), (1,-1,1),$

$(-1,1,1)$ and $(1,1,1)$ is the constant diagonal element $d_f = 0.7972$, of the hat matrix. Associated with the 6 axial points $(1,0,0), (-1,0,0), (0,1,0), (0,-1,0), (0,0,1)$ and $(0,0,-1)$ is the constant diagonal element $d_a = 0.5556$, of the hat matrix. Associated with the center point $(0,0,0)$ is the constant diagonal element $d_c = 0.2889$, of the hat matrix.

For a 7-parameter reduced second-order model in three control variables

$$y(x_1, x_2, x_3) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{11}x_1^2 + \epsilon$$

the hat matrix associated with central composite design having 8 factorial points, 6 axial points and 1 center point, is given as

$H =$

0.6500	-0.0500	0.2000	-0.0000	0.2000	-0.0000	-0.2500	0.0500	-0.0000	0.2000	-0.1000	0.1000	-0.1000	0.1000	0
-0.0500	0.6500	-0.0000	0.2000	-0.0000	0.2000	0.0500	-0.2500	0.2000	-0.0000	-0.1000	0.1000	-0.1000	0.1000	0
0.2000	-0.0000	0.6500	-0.0500	-0.2500	0.0500	0.2000	-0.0000	-0.0000	0.2000	0.1000	-0.1000	-0.1000	0.1000	0
-0.0000	0.2000	-0.0500	0.6500	0.0500	-0.2500	-0.0000	0.2000	0.2000	-0.0000	0.1000	-0.1000	-0.1000	0.1000	0
0.2000	-0.0000	-0.2500	0.0500	0.6500	-0.0500	0.2000	-0.0000	-0.0000	0.2000	-0.1000	0.1000	0.1000	-0.1000	0
-0.0000	0.2000	0.0500	-0.2500	-0.0500	0.6500	-0.0000	0.2000	0.2000	-0.0000	-0.1000	0.1000	0.1000	-0.1000	0
-0.2500	0.0500	0.2000	-0.0000	0.2000	-0.0000	0.6500	-0.0500	-0.0000	0.2000	0.1000	-0.1000	0.1000	-0.1000	0
0.0500	-0.2500	-0.0000	0.2000	-0.0000	0.2000	-0.0500	0.6500	0.2000	-0.0000	0.1000	-0.1000	0.1000	-0.1000	0
-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	0.2000	-0.0000	0	0	0	0	0
0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	0.2000	-0.0000	-0.0000	0.2000	0	0	0	0	0
-0.1000	-0.1000	0.1000	0.1000	-0.1000	-0.1000	0.1000	0.1000	0	0	0.3000	0.1000	0.2000	0.2000	0.2000
0.1000	0.1000	-0.1000	-0.1000	0.1000	0.1000	-0.1000	-0.1000	0	0	0.1000	0.3000	0.2000	0.2000	0.2000
-0.1000	-0.1000	-0.1000	-0.1000	0.1000	0.1000	0.1000	0.1000	0	0	0.2000	0.2000	0.3000	0.1000	0.2000
0.1000	0.1000	0.1000	0.1000	-0.1000	-0.1000	-0.1000	-0.1000	0	0	0.2000	0.2000	0.1000	0.3000	0.2000
0	0	0	0	0	0	0	0	0	0	0.2000	0.2000	0.2000	0.2000	0.2000

Associated with the 8 factorial points (-1,-1,-1), (1,-1,-1), (-1,1,-1), (1,1,-1), (-1,-1,1), (1,-1,1), (-1,1,1) and (1,1,1) is the constant diagonal element, $d_f = 0.6500$, of the hat matrix. Associated with the axial points are non-constant diagonal elements 0.2000 and 0.3000, of the hat matrix. Specifically, the points (1,0,0) and (-1,0,0) have same diagonal elements 0.2000 and the points (0,1,0), (0,-1,0), (0,0,1) and (0,0,-1) have same diagonal elements 0.3000. Associated with the center point (0,0,0) is the constant diagonal element $d_c = 0.2000$. Although each factorial point has same impact on modeling, influence due to axial points varies for some design points in the axial portion. Investigation into such points differing in impact may help in improving statistical estimations and establishing optimality measures and design efficiencies.

4. Construction of the Proposed Modified Central Composite Design (MCCD)

In the study of robustness against many cases of potential model mis-specification, central composite design is reported to be robust against model mis-specification in comparison to the Box-Behnken design as in Borkowski and Valeroso (1997). Myer *et al.* (2009) also observed the robustness of central composite design in relation to computer generated optimal design. For the purpose of illustrating the construction of Modified Central Composite Design, non-standard models may be formed using the following Hierarchical approach of Borkowski and Valeroso (1997): (i) If a model contains x_i^2 term, then it must contain the corresponding x_i term. (ii) If a model contains $x_i x_j$ term, then it must contain the corresponding x_i and / or x_j term. The central composite design shall be employed in the construction of optimal design for non-standard models. However adjustments will be made to eliminate points in CCD portions having low impacts on modeling. By classifying the diagonal element in the CCD portions, where there are non-constant diagonal elements (multiple influences or even losses) associated with a specific CCD portion, the design points having less influence may be deleted from the full CCD. This allows an improvement in design’s efficiency and offers alternative designs, similar in the structure of CCDs, for non-standard models. It is important to say at this juncture that the presence of no outlying observations is assumed.

5. Design Efficiency for Modified Central Composite Design on Non-standard Model

The design’s properties for the modified central composite design shall be considered by computing measures of design efficiencies. Commonly encountered efficiency measures include D- and G- efficiencies. For each reduced model considered, D-efficiency of the modified central composite design (MCCD) shall be compared with D-efficiency of the full central composite design (CCD). Similarly, G-efficiency of the modified central composite design shall be compared with G-efficiency of the full central composite design. As with its name, D-efficiency is a function of the D-optimality criterion which aims at minimizing the determinant of the variance-covariance matrix. On the other hand, G-efficiency is a function of the G-optimality criterion which as a minimax criterion aims at minimizing the maximum scaled prediction variance. By definition, D- and G-efficiency of a design are respectively

$$\text{D-efficiency} = 100 \left(\frac{|X'X|^{1/p}}{N} \right)$$

and

$$G\text{-efficiency} = 100 \left(\frac{p}{NSPV_{max}} \right)$$

where N is the design size, p is the number of model parameters, X is the model matrix and SPV_{max} is the maximum scaled prediction variance defined as in Myer *et al.* (2009). The computations of design efficiencies require that the optimal D and G values must be obtained.

6. Examples

Illustrations will be presented for design categories:

- (i) A CCD and a modified CCD in a cuboidal region for a non-standard model.
- (ii) A CCD and a modified CCD in a spherical region for a non-standard model.

The cuboidal region is typified by the choice of axial distance $\alpha = 1.0$ and the spherical region is typified by the choice of axial distance $\alpha = \sqrt{k}$ or $\alpha = (\sqrt{F})^{\frac{1}{4}}$ where k is the number of design variables and F is the number of factorial points in the design. The design efficiency measures shall be employed in assessing the full CCD and the modified CCD across the set of reduced models. However for completeness of comparisons, information regarding the full model shall also be presented.

Illustrations on Cuboidal Region

Example 1

The illustration considers the respective three-variable prior and posterior models

$$y(x_1, x_2, x_3) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{23}x_2x_3 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \beta_{33}x_3^2 + \epsilon$$

and

$$y(x_1, x_2, x_3) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{11}x_1^2 + \epsilon$$

defined on cuboidal region with axial distance $\alpha = 1.0$. The full CCD with one center point is

$$\xi_{15} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

The hat matrices associated with the designs for both prior and posterior models have been presented in section 3 and are in this illustration referred. With regards to the prior model, the model matrix for the full CCD is of dimension (15x10), where the number 15 represents the design size and the number 10 represents the total model parameters. The determinant value associated with the normalized information matrix is 3.1964×10^{-4} . The maximum scaled prediction variance is 11.9583. If the full CCD is defined in relation to the posterior model, the model matrix is the (15x7) matrix given below.

$$X_{15 \times 7} = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & -1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The determinant value of normalized information matrix associated with the complete design for the posterior model is 0.0185. The maximum scaled prediction variance is 9.75. Upon examination of the hat matrix associated with the posterior model, the design points (1, 0, 0) and (-1, 0, 0) are deleted from the complete design. This gives a reduction in the size of the design and a resulting 13-point design emerges. Thus, the modified CCD for the posterior model is

$$\xi_{13} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 0 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

The (13x7) associated model matrix is

$$X_{13 \times 7} = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The determinant value of normalized information matrix is 0.0326. The maximum scaled prediction variance is 9.1000. The optimality measures and efficiency values for the full and modified CCDs associated with the prior and posterior models are summarized in Table 1.

Table 1. Optimality measures and efficiency values for full and modified CCDs ($k=3, n_c = 1, \alpha=1$)

Three Control Variables ($\alpha=1.0$)	Determinant Value	D-efficiency	Maximum SPV	G-efficiency
Full model, Full CCD, p=10	3.1964x10	44.72%	11.9583	83.62%
Reduced Model, Full CCD, p=7	0.0185	59.64%	9.75	71.79%
Reduced Model M CCD, p=7	0.0326	61.32%	9.1000	76.92%

Example 2

The illustration considers the respective four-variable prior and posterior models

$$y(x_1, x_2, x_3, x_4) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{14}x_1x_4 + \beta_{23}x_2x_3 + \beta_{24}x_2x_4 + \beta_{34}x_3x_4 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \beta_{33}x_3^2 + \beta_{44}x_4^2 + \varepsilon$$

and

$$y(x_1, x_2, x_3, x_4) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{12}x_1x_2 + \beta_{23}x_2x_3 + \beta_{11}x_1^2 + \beta_{44}x_4^2 + \varepsilon$$

defined on cuboidal region with axial distance $\alpha = 1.0$. The full CCD with one center point is

$$\xi_{25} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

With regards to the prior model, the model matrix for the full CCD is of dimension (25x15). The columns of the hat matrix associated with the full model are as in Appendix A. The determinant value of normalized information matrix associated with the complete design for the prior model is 5.3555×10^{-6} . The maximum scaled prediction variance is 16.4842.

The design matrix associated with the 9-parameter posterior model is given as

$X_{25 \times 9} =$

1	-1	-1	-1	-1	1	1	1	1
1	1	-1	-1	-1	-1	1	1	1
1	-1	1	-1	-1	-1	-1	1	1
1	1	1	-1	-1	1	-1	1	1
1	-1	-1	1	-1	1	-1	1	1
1	1	-1	1	-1	-1	-1	1	1
1	-1	1	1	-1	-1	1	1	1
1	1	1	1	-1	1	1	1	1
1	-1	-1	-1	1	1	1	1	1
1	1	-1	-1	1	-1	1	1	1
1	-1	1	-1	1	-1	-1	1	1
1	1	1	-1	1	1	-1	1	1
1	-1	-1	1	1	1	-1	1	1
1	1	-1	1	1	-1	-1	1	1
1	-1	1	1	1	-1	1	1	1
1	1	1	1	1	1	1	1	1
1	1	0	0	0	0	0	1	0
1	-1	0	0	0	0	0	1	0
1	0	1	0	0	0	0	0	0
1	0	-1	0	0	0	0	0	0
1	0	0	1	0	0	0	0	0
1	0	0	-1	0	0	0	0	0
1	0	0	0	1	0	0	0	1
1	0	0	0	-1	0	0	0	1
1	0	0	0	0	0	0	0	0

The determinant value of normalized information matrix associated with the complete design for the prior model is 0.0028. The maximum scaled prediction variance is 10.1657. Upon examination of the hat matrix in Appendix B associated with the posterior model, the design points (0, 1, 0, 0), (0, -1, 0, 0), (0, 0, 1, 0) and (0, 0, -1, 0) are deleted from the complete design. This gives a reduction in the size of the design and a resulting 21-point design emerges. Thus, the modified CCD for the posterior model is

$$\xi_{21} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The (21x9) associated model matrix is

$$X_{21 \times 9} = \begin{pmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The determinant value of normalized information matrix is 0.0035. The maximum scaled prediction variance is 10.8182. The optimality measures and efficiency values for the full and modified CCDs associated with the prior and posterior models are summarized in Table 2.

Table 2 Optimality measures and efficiency values for full and modified CCDs ($k=4, n_c = 1, \alpha=1$)

Four Control Variables ($\alpha=1.0$)	Determinant Value	D-efficiency	Maximum SPV	G-efficiency
Full model, Full CCD, p=15	5.3555×10^{-6}	44.52%	16.4842	91.00%
Reduced Model, Full CCD, p=9	0.0028	52.04%	10.1657	88.53%
Reduced Model MCCD, p=9	0.0035	53.35%	10.8182	83.19%

Illustrations on spherical region

Example 3

The illustration considers the respective three-variable prior and posterior models

$$y(x_1, x_2, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \epsilon$$

and

$$y(x_1, x_2, x_3) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \beta_{11} x_1^2 + \epsilon$$

defined on spherical region with axial distance $\alpha = \sqrt{3} = 1.732$. The full CCD with four center points is

$$\xi_{18} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1.7321 & 0 & 0 \\ -1.7321 & 0 & 0 \\ 0 & 1.7321 & 0 \\ 0 & -1.7321 & 0 \\ 0 & 0 & 1.7321 \\ 0 & 0 & -1.7321 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

With regards to the prior model, the model matrix for the full CCD is of dimension (18x10). The columns of the hat matrix associated with the full model are as in Appendix C. The determinant value of normalized information matrix associated with the complete design for the prior model is 0.0214. The maximum scaled prediction variance is 11.8927.

The design matrix associated with the 8-parameter posterior model is given as

$$X_{18 \times 8} = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1.7321 & 0 & 0 & 0 & 0 & 0 & 3.0002 \\ 1 & -1.7321 & 0 & 0 & 0 & 0 & 0 & 3.0002 \\ 1 & 0 & 1.7321 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & -1.7321 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1.7321 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -1.7321 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The determinant value of normalized information matrix associated with the complete design for the posterior model is 0.0347. The maximum scaled prediction variance is 11.6659. Upon examination of the hat matrix in Appendix D associated with the posterior model, the design points (0, 1.7321, 0), (0, -1.7321, 0), (0, 0, 1.7321) and (0, 0, -1.7321) are deleted from the complete design. This gives a reduction in the size of the design and a resulting 14-point design emerges. Thus, the modified CCD for the posterior model is

$$\xi_{14} = \begin{pmatrix} -1 & -1 & -1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 1 & 1 \\ 1.7321 & 0 & 0 \\ -1.7321 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The (14x8) associated model matrix is

$$X_{14 \times 8} = \begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1.7321 & 0 & 0 & 0 & 0 & 0 & 3.0002 \\ 1 & -1.7321 & 0 & 0 & 0 & 0 & 0 & 3.0002 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The determinant value of normalized information matrix is 0.0522. The maximum scaled prediction variance is 10.7500. The optimality measures and efficiency values for the full and modified CCDs associated with the prior and posterior models are summarized in Table 3.

Table 3. Optimality measures and efficiency values for full and modified CCDs ($k=3, n_c = 4, \alpha = 1.7321$)

Three Control Variables $\alpha=1.7321$	Maximum Det. Value	D- Efficiency	Maximum SPV	G-Efficiency
Full model, full CCD, $p=10$	0.0214	68.08%	11.8927	84.09%
Reduced Model, full CCD $p = 8$	0.0347	65.70%	11.6659	68.58%
Reduced Model M CCD $p = 8$	0.0522	69.14%	10.7500	74.42%

Example 4

The illustration considers the respective four-variable prior and posterior models

$$y(x_1, x_2, x_3, x_4) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{14}x_1x_4 + \beta_{23}x_2x_3 + \beta_{24}x_2x_4 + \beta_{34}x_3x_4 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \beta_{33}x_3^2 + \beta_{44}x_4^2 + \varepsilon$$

and

$$y(x_1, x_2, x_3, x_4) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{14}x_1x_4 + \beta_{23}x_2x_3 + \beta_{24}x_2x_4 + \beta_{34}x_3x_4 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \varepsilon$$

defined on spherical region with axial distance $\alpha = (2^k)^{\frac{1}{4}} = 2.0$. The full CCD with one center point is

$$\xi_{25} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 2 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

With regards to the prior model, the model matrix for the full CCD is of dimension (25x15). The columns of the hat matrix

associated with the full model are as in Appendix E. The determinant value of normalized information matrix associated with the complete design for the prior model is 0.0188. The maximum scaled prediction variance is 25.0.

The design matrix associated with the 13-parameter posterior model is given as

$$X_{25 \times 13} = \begin{pmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \\ 1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \\ 1 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The determinant value of normalized information matrix associated with the complete design for the posterior model is 0.0536. The maximum scaled prediction variance is 14.5461. Upon examination of the hat matrix in Appendix F associated with the posterior model, the design points (0, 0, 2, 0), (0, 0, -2, 0), (0, 0, 0, 2) and (0, 0, 0, -2) are deleted from the complete design. This gives a reduction in the size of the design and a resulting 21-point design emerges. Thus, the modified CCD for the posterior model is

$$\xi_{21} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 2 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The (21x13) associated model matrix is

$$X_{21 \times 13} = \begin{pmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \\ 1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The determinant value of normalized information matrix is 0.0984. The maximum scaled prediction variance is 13.3438. The optimality measures and efficiency values for the full and modified CCDs associated with the prior and posterior models are summarized in Table 4.

Table 4. Optimality measures and efficiency values for full and modified CCDs ($k=4, n_c = 1, \alpha = 2.0$)

Four Control Variables $\alpha=2$	Maximum Det. Value	D- Efficiency	Maximum SPV	G-Efficiency
Full model, full CCD, p =15	0.0188	76.73%	25.0000	60.00%
Reduced Model, full CCD p =13	0.0536	79.84%	14.5461	89.37%
Reduced Model M CCD p =13	0.0984	83.66%	13.3438	97.42%

Example 5

The illustration considers the respective four-variable prior and posterior models

$$y(x_1, x_2, x_3, x_4) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{14}x_1x_4 + \beta_{23}x_2x_3 + \beta_{24}x_2x_4 + \beta_{34}x_3x_4 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \beta_{33}x_3^2 + \beta_{44}x_4^2 + \varepsilon$$

and

$$y(x_1, x_2, x_3, x_4) = \beta_0 + \beta_1x_1 + \beta_2x_2 + \beta_3x_3 + \beta_4x_4 + \beta_{12}x_1x_2 + \beta_{13}x_1x_3 + \beta_{14}x_1x_4 + \beta_{23}x_2x_3 + \beta_{24}x_2x_4 + \beta_{34}x_3x_4 + \beta_{11}x_1^2 + \beta_{22}x_2^2 + \varepsilon$$

defined on spherical region with axial distance $\alpha = (2^k)^{\frac{1}{4}} = 2.0$. The full CCD with three center points is

$$\xi_{27} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 2 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & -2 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

With regards to the prior model, the model matrix for the full CCD is of dimension (27x15). The columns of the hat matrix associated with the full model are as in Appendix G. The determinant value of normalized information matrix associated with the complete design for the prior model is 0.0178. The maximum scaled prediction variance is 15.75.

The design matrix associated with the 13-parameter posterior model is given as

$$X_{27 \times 13} = \begin{pmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \\ 1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \\ 1 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The determinant value of normalized information matrix associated with the complete design for the posterior model is 0.0253. The maximum scaled prediction variance is 15.6563. Upon examination of the hat matrix in Appendix H associated with the posterior model, the design points (0, 0, 2, 0), (0, 0, -2, 0), (0, 0, 0, 2) and (0, 0, 0, -2) are deleted from the complete design. This gives a reduction in the size of the design and a resulting 21-point design emerges. Thus, the modified CCD for the posterior model is

$$\xi_{23} = \begin{pmatrix} -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 2 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The (23x13) associated model matrix is

$$X_{23 \times 13} = \begin{pmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & -1 & 1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ 1 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \\ 1 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

The determinant value of normalized information matrix is 0.0503. The maximum scaled prediction variance is 14.4229. The optimality measures and efficiency values for the full and modified CCDs associated with the prior and posterior models are summarized in Table 5.

Table 5. Optimality measures and efficiency values for full and modified CCDs ($k=4, n_c = 3, \alpha = 2.0$)

Four Control Variables $\alpha=2$	Maximum Det. Value	D- Efficiency	Maximum SPV	G-Efficiency
Full model, full CCD, $p = 15$	0.0178	76.45%	15.7500	95.24%
Reduced Model, full CCD $p = 13$	0.0253	75.36%	15.6563	83.03%
Reduced Model MCCD $p = 13$	0.0503	79.45%	14.4229	90.13%

7. Discussion of Results

The removal of less influential design points in the axial portion of the central composite design generally improves the efficiency of the design. For a three-variable central composite design having one center point and defined for $\alpha = 1.0$, the D-efficiency of the CCD defined for a complete prior 10-parameter model is not as high as the D-efficiency of the CCD defined for the 7-parameter posterior model. The D-efficiency of the modified central composite design for the posterior model exceeds the D-efficiency of the complete CCD whether it is defined for the prior or posterior model. Also, the G-efficiency associated with the modified central composite design defined for the posterior model exceeds the G-efficiency associated with the complete CCD defined for the posterior model. However, the G-efficiency associated with the complete central composite design defined for the prior model exceeds the G-efficiency associated with the

complete and modified CCDs defined for the posterior model. What stands out prominently is that G-efficiency values in all three specifications exceed the D-efficiency values.

For the four-variable central composite design having one center point and defined for $\alpha = 1.0$, the result is similar in the structure of D-efficiency as in the three-variable case, having one center point and defined for $\alpha = 1.0$. Specifically, the D-efficiency of the CCD defined for a complete prior 15-parameter model is not as high as the D-efficiency of the CCD defined for the 9-parameter posterior model. The D-efficiency of the modified central composite design for the posterior model exceeds the D-efficiency of the complete CCD whether it is defined for the prior or posterior model. On the other hand however, the complete CCD defined for the posterior model has slightly higher G-efficiency value than the G-efficiency value associated with the modified central composite design for the posterior model. Again, as in the three-variable case, the G-efficiency values associated with the complete and modified CCDs are higher than the corresponding D-efficiency values whether prior or posterior models are in use.

For a three-variable central composite design having four center points and defined for $\alpha = 1.7321$, the D-efficiency of the complete CCD defined for a complete prior 10-parameter model is not as high as the D-efficiency of the modified CCD defined for the 8-parameter posterior model even though it is higher than the D-efficiency of the complete central composite design defined for the posterior model. The G-efficiency associated with the modified central composite design defined for the posterior model exceeds the G-efficiency associated with the complete CCD defined for the posterior model. However, the G-efficiency associated with the complete central composite design defined for the prior model exceeds the G-efficiency associated with the complete and modified CCDs defined for the posterior model. What again stands out prominently is that G-efficiency values in all three specifications exceed the D-efficiency values.

For the four-variable central composite design having one center point and defined for $\alpha = 2.0$, both D- and G-efficiency values associated with the modified CCD defined for the posterior 13-parameter posterior model exceed the D- and G-efficiency values associated with the complete CCD defined for either the 15-parameter prior model or the 13-parameter posterior model. G-efficiency values associated with the complete and modified CCDs are higher than the corresponding G-efficiency values when defined for the 13-parameter posterior model. An exception holds for the complete CCD defined on the 15-parameter prior model, where the G-efficiency value is less than the corresponding D-efficiency value.

For the four-variable central composite design having three center points and defined for $\alpha = 2.0$, the D-efficiency of the modified central composite design for the 13-parameter posterior model exceeds the D-efficiency of the complete CCD whether it is defined for the 15-parameter prior or for the 13-parameter posterior model. Also, the G-efficiency value associated with the modified central composite design for the 13-parameter posterior model is higher than the G-efficiency value associated with the complete CCD defined for the 13-parameter posterior model. In all three cases, the G-efficiency values associated with the complete and modified CCDs are higher than the corresponding D-efficiency values whether prior or posterior models are in use.

8. Conclusion

Designs for non-standard models are constructed using principles of the loss function. The designs are a modification of central composite designs and are similar in the structure of CCDs. By studying possible losses due to missing design points in the CCD portions, where there are multiple losses associated with specified CCD portions, the design points having less influence may be deleted from the full CCD. This leads to a possible increase in design efficiency and offers alternative designs, similar in the structure of CCDs, for non-standard models.

References

- Ahmad, T., & Gilmour, S. G. (2010). Robustness of subset response surface designs to missing observations. *Journal of Statistical Planning and Inference*, 140(1), 92-103.
- Ahmad, T., Akhtar, M., & Gilmour, S. G. (2012). Multilevel augmented pairs second-order response surface designs and their robustness to missing data. *Communications in Statistics-Theory and Methods*, 41(3), 437-452.
- Akhtar, M. (1987). One or two missing observations in five factor Box and Behnken design. *Journal of Engg. & App. Scs.* 6(1), 87-89.
- Akhtar, M. (2001). Five-factor central composite designs robust to a pair of missing observations. *J. Res. Sci*, 12(2), 105-115.
- Akhtar, M., & Prescott, P. (1986). Response surface designs robust to missing observations. *Communications in Statistics-Simulation and Computation*, 15(2), 345-363.
- Akram, M. (2002). Central composite designs robust to three missing observations, doctorate. *The Islamia University Bahawalpur, Pakistan*.

APPENDIX C: HAT MATRIX full CCD, Prior Model , k=3 defined on spherical region with axial distance

$\alpha = \sqrt{3} = 1.7321$ and four center points

Table with 16 columns and 40 rows of numerical data representing the HAT matrix for k=3.

APPENDIX D: HAT MATRIX full CCD, Posterior Model , k=3 defined on spherical region with axial distance

$\alpha = \sqrt{3} = 1.7321$ and four center points

Table with 16 columns and 40 rows of numerical data representing the HAT matrix for k=3 in the posterior model.

APPENDIX E: HAT MATRIX full CCD, Prior Model, k=4 defined on spherical region with axial distance

$\alpha = (2^k)^{\frac{1}{4}} = 2.0$ and one center point

Table with 16 columns and 40 rows of numerical data representing the HAT matrix for k=4.

APPENDIX F: HAT MATRIX full CCD, Posterior Model, k=4 defined on spherical region with axial distance

alpha = (2^k)^(1/4) = 2.0 and one center point

Table with 13 columns of numerical values representing the HAT matrix for Appendix F.

APPENDIX G: HAT MATRIX full CCD, Prior Model, k=4 defined on spherical region with axial distance

alpha = (2^k)^(1/4) = 2.0 and three center points

Table with 13 columns of numerical values representing the HAT matrix for Appendix G.

APPENDIX H: HAT MATRIX full CCD, Posterior Model, k=4 defined on spherical region with axial distance

alpha = (2^k)^(1/4) = 2.0 and three center points

Table with 13 columns of numerical values representing the HAT matrix for Appendix H.

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